OpenCMISS-iron examples and tests used by OpenCMISS developers at University of Stuttgart, Germany

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INTRODUCTION 1

This document contains information about examples used for testing OpenCMISSiron. Read: How-to¹ and [1].

- Cmgui files for cmgui-2.9
- Variations to consider
 - Geometry and topology

1D, 2D, 3D

Length, width, height

Number of elements

Interpolation order

Generated or user meshes

quad/hex or tri/tet meshes

- Initial conditions
- Load cases

Dirichlet BC

Neumann BC

Volume force

Mix of previous items

- Sources, sinks
- Time dependence

Static

Quasi-static

Dynamic

Material laws

Linear

Nonlinear (Mooney-Rivlin, Neo-Hookean, Ogden, etc.)

Active (Stress, strain)

- Material parameters, anisotropy
- Solver

Direct

Iterative

Test cases

Numerical reference data

Analytical solution

• A mix of previous items

¹ https://bitbucket.org/hessenthaler/opencmiss-howto

1.3 Folder structure

TBD..

HOW TO WORK ON THIS DOCUMENT

In the Google Doc at https://docs.google.com/spreadsheets/d/1RGKj8vVPqQ-PH0UwMX_ e9TAzqaYavKi0z0D4pKY9RGI/edit#gid=0 please indicate what you are working on or if a given example was finished

- no mark: to be done
- x: currently working on it
- xx: done

Initials	Full name
СВ	Christian Bleiler
AH	Andreas Hessenthaler
TK	Thomas Klotz
AK	Aaron Krämer
BM	Benjamin Maier
SM	Sergio Morales
MM	Mylena Mordhorst
HS	Harry Saini

 Table 1: Initials of people working on examples, in alphabetical order (surnames).

3 DIFFUSION EQUATION

3.1 Equation in general form

The governing equation is,

$$\partial_t \mathbf{u} + \nabla \cdot [\boldsymbol{\sigma} \nabla \mathbf{u}] = \mathbf{f}, \tag{1}$$

with conductivity tensor $\boldsymbol{\sigma}.$ The conductivity tensor is,

- defined in material coordinates (fibre direction),
- diagonal,
- defined per element.

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.2.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{2}$$

with boundary conditions

$$u = 0 x = y = 0, (3)$$

$$u = 1$$
 $x = 2, y = 1.$ (4)

No material parameters to specify.

3.2.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{5}$$

with boundary conditions

$$u = 0 \qquad \qquad x = y = z = 0, \tag{6}$$

$$u = 1$$
 $x = 2, y = z = 1.$ (7)

No material parameters to specify.

3.2.3 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

• Commandline arguments for tests are:

2.0 1.0 0.0 2 1 0 1 0

2.0 1.0 0.0 4 2 0 1 0

2.0 1.0 0.0 8 4 0 1 0

2.0 1.0 0.0 2 1 0 2 0

2.0 1.0 0.0 4 2 0 2 0

2.0 1.0 0.0 8 4 0 2 0

2.0 1.0 0.0 2 1 0 1 1

2.0 1.0 0.0 4 2 0 1 1

3.2.4 Result summary

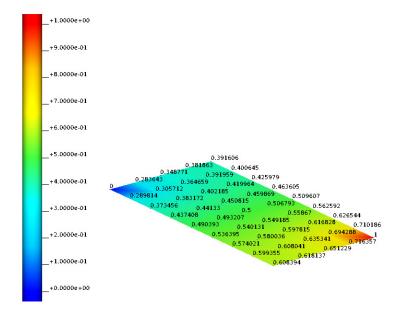


Figure 1: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1

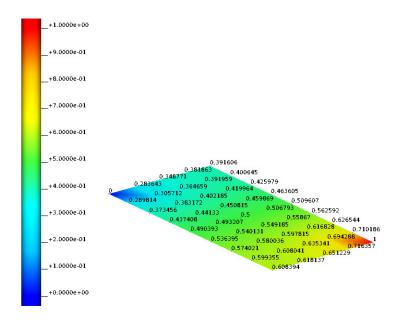


Figure 2: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

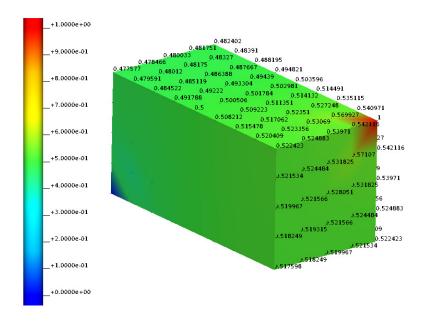


Figure 3: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 o].

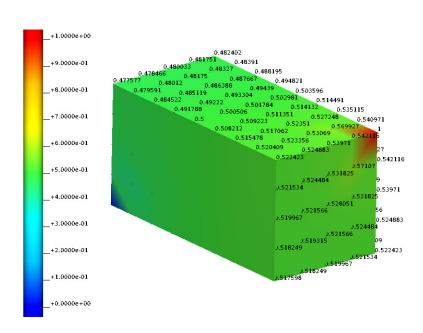


Figure 4: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

3.3 Example-0001-u

Example uses user-defined regular meshes in CHeart mesh format and solves a static problem, i.e., applies the boundary conditions in one step.

3.3.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{8}$$

with boundary conditions

$$u = 0 x = y = 0, (9)$$

$$u = 1$$
 $x = 2, y = 1.$ (10)

No material parameters to specify.

3.3.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{11}$$

with boundary conditions

$$u = 0 \qquad \qquad x = y = z = 0, \tag{12}$$

$$u = 1$$
 $x = 2, y = z = 1.$ (13)

No material parameters to specify.

3.3.3 Computational model

Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

Commandline arguments for tests are:

2.0 1.0 0.0 2 1 0 1 0

2.0 1.0 0.0 4 2 0 1 0

2.0 1.0 0.0 8 4 0 1 0

2.0 1.0 0.0 2 1 0 2 0

2.0 1.0 0.0 4 2 0 2 0

2.0 1.0 0.0 8 4 0 2 0

2.0 1.0 0.0 2 1 0 1 1

2.0 1.0 0.0 4 2 0 1 1

```
2.0 1.0 0.0 8 4 0 1 1
2.0 1.0 0.0 2 1 0 2 1
2.0 1.0 0.0 4 2 0 2 1
2.0 1.0 0.0 8 4 0 2 1
2.0 1.0 1.0 2 1 1 1 0
2.0 1.0 1.0 4 2 2 1 0
2.0 1.0 1.0 8 4 4 1 0
2.0 1.0 1.0 2 1 1 2 0
2.0 1.0 1.0 4 2 2 2 0
2.0 1.0 1.0 8 4 4 2 0
2.0 1.0 1.0 2 1 1 1 1
2.0 1.0 1.0 4 2 2 1 1
2.0 1.0 1.0 8 4 4 1 1
2.0 1.0 1.0 2 1 1 2 1
2.0 1.0 1.0 4 2 2 2 1
2.0 1.0 1.0 8 4 4 2 1
```

• Note: Binary uses command line arguments to search for the relevant mesh files.

3.3.4 Result summary

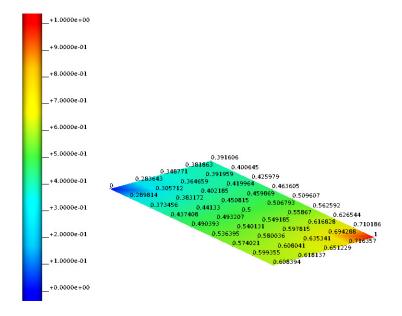


Figure 5: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 o].

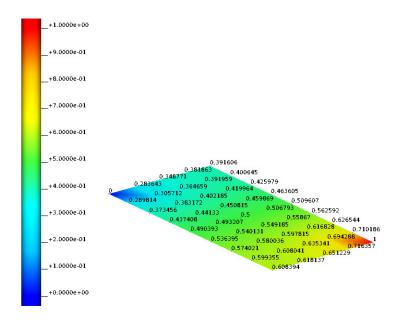


Figure 6: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

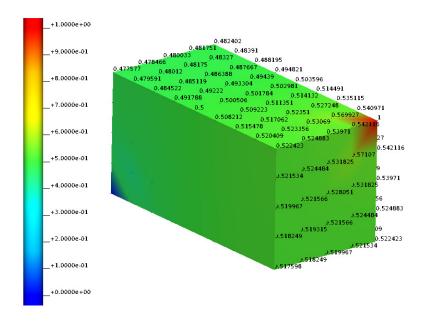


Figure 7: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 o].

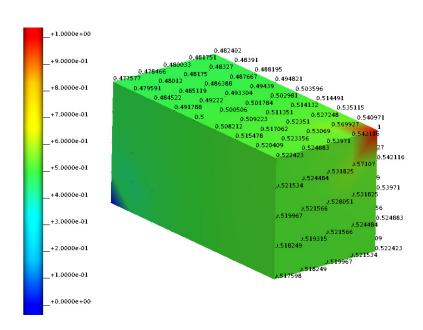


Figure 8: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

3.4 Example-0002

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.4.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = \mathbf{0} \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{14}$$

with boundary conditions

$$u = 15y$$
 $x = 0$, (15)

$$u = 25 - 18y$$
 $x = 2.$ (16)

No material parameters to specify.

3.4.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = \mathbf{0} \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{17}$$

with boundary conditions

$$u = 15y x = 0, (18)$$

$$u = 25 - 18y$$
 $x = 2.$ (19)

No material parameters to specify.

3.4.3 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

Commandline arguments for tests are:

2.0 1.0 0.0 2 1 0 1 0

2.0 1.0 0.0 4 2 0 1 0

2.0 1.0 0.0 8 4 0 1 0

2.0 1.0 0.0 2 1 0 2 0

2.0 1.0 0.0 4 2 0 2 0

2.0 1.0 0.0 8 4 0 2 0

2.0 1.0 0.0 2 1 0 1 1

2.0 1.0 0.0 4 2 0 1 1

3.4.4 Result summary

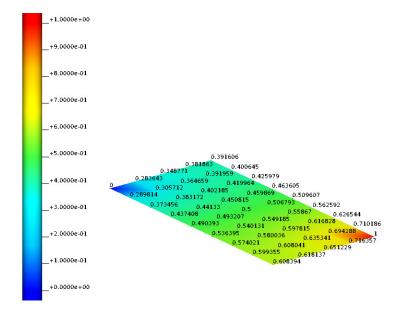


Figure 9: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1

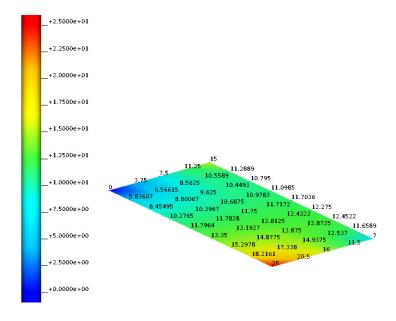


Figure 10: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 $\,$ o].

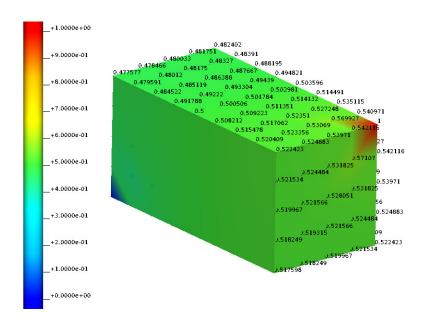


Figure 11: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 10].

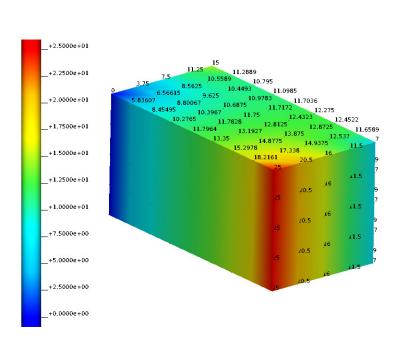


Figure 12: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 o].

3.5 Example-0003

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.5.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{20}$$

with boundary conditions

$$u = 15y \qquad x = 0, \tag{21}$$

$$u = 15y$$
 $x = 0,$ (21) $\vartheta_n u = 25 - 18y$ $x = 2.$ (22)

No material parameters to specify.

3.5.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{23}$$

with boundary conditions

$$u = 15y$$
 $x = 0$, (24)

$$\partial_n u = 25 - 18y$$
 $x = 2.$
(25)

No material parameters to specify.

3.5.3 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

Commandline arguments for tests are:

2.0 1.0 0.0 2 1 0 1 0

2.0 1.0 0.0 4 2 0 1 0

2.0 1.0 0.0 8 4 0 1 0

2.0 1.0 0.0 2 1 0 2 0

2.0 1.0 0.0 4 2 0 2 0

2.0 1.0 0.0 8 4 0 2 0

2.0 1.0 0.0 2 1 0 1 1

2.0 1.0 0.0 4 2 0 1 1

```
2.0 1.0 0.0 8 4 0 1 1
2.0 1.0 0.0 2 1 0 2 1
2.0 1.0 0.0 4 2 0 2 1
2.0 1.0 0.0 8 4 0 2 1
2.0 1.0 1.0 2 1 1 1 0
2.0 1.0 1.0 4 2 2 1 0
2.0 1.0 1.0 8 4 4 1 0
2.0 1.0 1.0 2 1 1 2 0
2.0 1.0 1.0 4 2 2 2 0
2.0 1.0 1.0 8 4 4 2 0
2.0 1.0 1.0 2 1 1 1 1
2.0 1.0 1.0 4 2 2 1 1
2.0 1.0 1.0 8 4 4 1 1
2.0 1.0 1.0 2 1 1 2 1
2.0 1.0 1.0 4 2 2 2 1
2.0 1.0 1.0 8 4 4 2 1
```

3.5.4 Result summary

Figure 13: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 10].

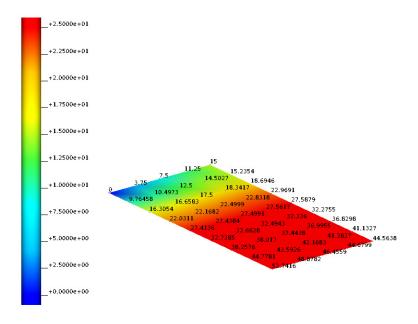


Figure 14: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1

Figure 15: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 $^{\circ}$ 10].

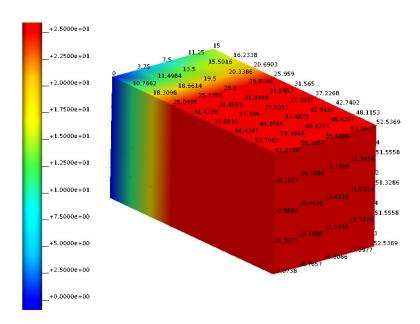


Figure 16: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 o].

3.6 Example-0004

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.6.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{26}$$

with boundary conditions

$$u = 2.0e^{x} \cdot \cos(y)$$
 on $\partial\Omega$. (27)

No material parameters to specify.

3.6.2 Computational model

• Commandline arguments are:

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

• Commandline arguments for tests are:

42010

84010

21020

42020

84020

42011

84011

21021

42021

84021

100 50 0 1 0 (not tested yet..)

100 50 0 2 0 (not tested yet..)

100 50 0 1 1 (not tested yet..)

100 50 0 2 1 (not tested yet..)

3.6.3 Result summary

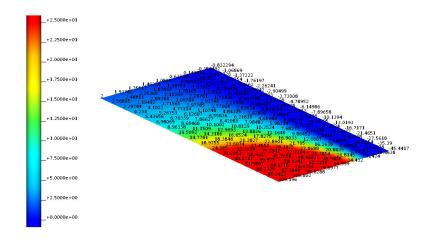


Figure 17: 2D results, iron reference w/ command line arguments [8 4 0 2 0].

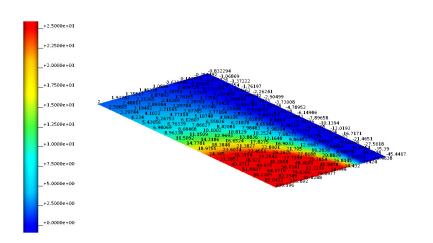


Figure 18: 2D results, current run w/ command line arguments [8 4 0 2 0].

3.7 Example-0011

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

3.7.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot [\sigma \nabla u] = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{28}$$

with boundary conditions

$$u = 0 x = y = 0, (29)$$

$$u = 1$$
 $x = 2, y = 1.$ (30)

The conductivity tensor is defined as,

$$\sigma(x,t) = \sigma = I. \tag{31}$$

3.7.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot [\boldsymbol{\sigma} \nabla \mathbf{u}] = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{32}$$

with boundary conditions

$$u = 0$$
 $x = y = z = 0,$ (33)

$$u = 1$$
 $x = 2, y = z = 1.$ (34)

The conductivity tensor is defined as,

$$\sigma(x,t) = \sigma = I. \tag{35}$$

3.7.3 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

integer: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

float: σ_{11} float: σ_{22}

float: σ_{33} (ignored for 2D)

• Commandline arguments for tests are:

3.7.4 Result summary

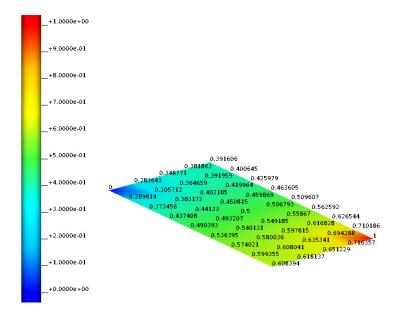


Figure 19: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1011].

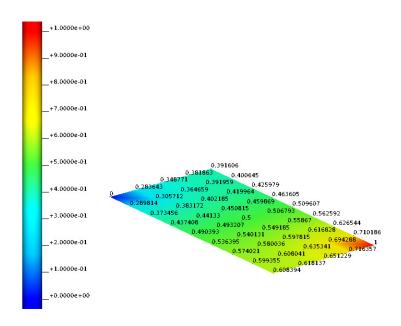


Figure 20: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0 1 1].

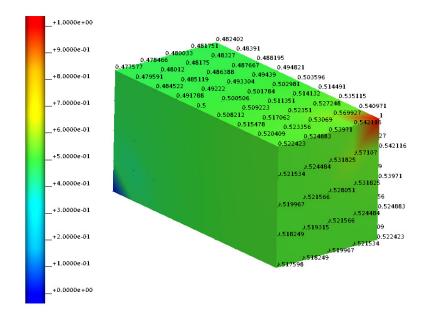


Figure 21: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 10111].

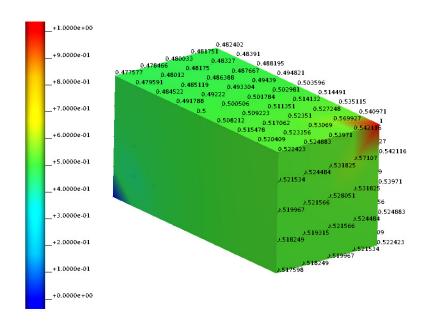


Figure 22: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0 1 1 1].

4 LINEAR ELASTICITY

4.1 Equation in general form

$$\partial_{tt} \mathbf{u} + \nabla \cdot \mathbf{\sigma}(\mathbf{u}, \mathbf{t}) = \mathbf{f}(\mathbf{u}, \mathbf{t}) \tag{36}$$

4.2 Example-0101

4.2.1 Mathematical model

We solve the following equation (both 2D and 3D domains are considered),

$$\nabla \cdot \sigma(\mathbf{u}, \mathbf{t}) = 0$$
 $\Omega = [0, 160] \times [0, 120] \times [0, 120], \mathbf{t} \in [0, 5],$ (37)

with time step size $\Delta_t = 1$ and $u = [u_x, u_y]$ in 2D $u = [u_x, u_y, u_z]$ in 3D. The boundary conditions in 2D are given by

$$u_x = u_y = 0 \qquad \qquad x = y = 0, \tag{38}$$

$$u_x = 16$$
 $x = 160$, (39)

and in 3D by

$$u_x = u_y = u_z = 0$$
 $x = y = z = 0$, (40)

$$u_x = 16$$
 $x = 160$. (41)

The material parameters are

$$E = 10000MPa,$$
 (42)

$$v = 0.3,$$
 (43)

$$\rho = 5 \times 10^{-9} \text{tonne.mm}^3. \tag{44}$$

4.2.2 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

integer: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

float: elastic modulus float: Poisson ratio

float: displacement percentage load

• Commandline arguments for tests are:

4.2.3 Results

4.2.4 Validation

CHeart rev. 6328, Abaqus 2017, analytical reference solution, whatever...

Figure 23: Results, analytical solution.

Figure 24: Results, Abaqus reference.

Figure 25: Results, iron reference.

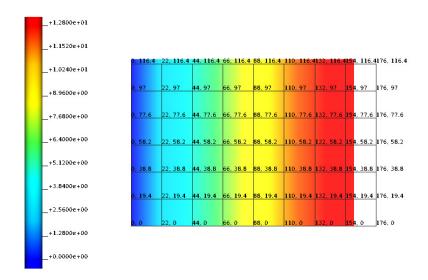


Figure 26: Results, current run.

4.3.1 Mathematical model

We solve the following equation (both 2D and 3D domains are considered),

$$\nabla \cdot \sigma(\mathbf{u}, \mathbf{t}) = 0$$
 $\Omega = [0, 160] \times [0, 120] \times [0, 120], \mathbf{t} \in [0, 5],$ (45)

with time step size $\Delta_t = 1$ and $\mathbf{u} = [u_x, u_y]$ in 2D $\mathbf{u} = [u_x, u_y, u_z]$ in 3D. The boundary conditions in 2D are given by

$$u_{x} = u_{y} = 0 \qquad \qquad y = 0, \tag{46}$$

$$u_y = 8$$
 $x = 160,$ (47)

and in 3D by

$$u_x = u_z = 0 x = 0, (48)$$

$$u_y = 0 y = 0, (49)$$

$$u_x = 160$$
 $x = 160$, (50)

$$u_y = 8$$
 $x = 160.$ (51)

The material parameters are

$$E = 10000MPa,$$
 (52)

$$v = 0.3, \tag{53}$$

$$\rho = 5 \times 10^{-9} \text{tonne.mm}^3. \tag{54}$$

4.3.2 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

integer: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

float: elastic modulus float: Poisson ratio

float: displacement percentage load

• Commandline arguments for tests are:

• • •

4.3.3 Results

4.3.4 Validation

CHeart rev. 6328, Abaqus 2017, analytical reference solution, whatever...

Figure 27: Results, analytical solution.

Figure 28: Results, Abaqus reference.

Figure 29: Results, iron reference.

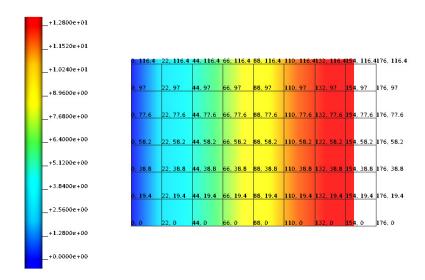


Figure 30: Results, current run.

5 FINITE ELASTICITY

6 NAVIER-STOKES FLOW

6.1 Equation in general form

$$\partial_{\mathbf{t}}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + p\mathbf{I}) = \rho \mathbf{f}$$
 (55)

6.2 Example-0302-u

Example uses user-defined regular meshes in CHeart mesh format with quadratic- linear interpolation for velocity-pressure and solves a dynamic problem.

6.2.1 Mathematical model - 2D

We solve the incompressible Navier-Stokes equation,

$$\partial_{\mathbf{t}}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + \rho \mathbf{I}) = \rho \mathbf{f} \qquad \qquad \Omega = [0, 1] \times [0, 1], \qquad (56)$$

$$\nabla \cdot \mathbf{v} = 0, \qquad (57)$$

with boundary conditions

$$u = 0$$
 $x = 0$, (58)
 $u = 0$ $x = 1$, (59)
 $u = 0$ $y = 0$, (60)
 $u = 1$ $y = 1$. (61)

Density $\rho = 1$, viscosity $\mu = 0.0025$. Thus, Reynolds number Re = 400.

6.2.2 Mathematical model - 3D

We solve the incompressible Navier-Stokes equation,

$$\partial_{\mathsf{t}}(\rho \nu) + \nabla \cdot (\rho \nu \otimes \nu + p\mathbf{I}) = \rho \mathbf{f} \qquad \Omega = [0, 1] \times [0, 1] \times [0, 1], \tag{62}$$
$$\nabla \cdot \nu = 0, \tag{63}$$

with boundary conditions

$$u = 0$$
 $x = 0$, (64)

 $u = 0$
 $x = 1$, (65)

 $u = 0$
 $y = 0$, (66)

 $u = 1$
 $y = 1$, (67)

 $u = 0$
 $z = 0$, (68)

 $u = 0$
 $z = 1$, (69)

Density $\rho = 1$, viscosity $\mu = 0.01$. Thus, Reynolds number Re = 100.

6.2.3 Computational model

• Commandline arguments are:

integer: number of dimensions (2: 2D, 3: 3D integer: mesh refinement level (1, 2, 3, ...)

float: start time float: stop time float: time step size float: density

float: viscosity

integer: solver type (o: direct; 1: iterative)

- Commandline arguments for tests are:
 - 2 1 0.0 0.01 0.001 1.0 0.0025 0
- Note: Binary uses command line arguments to search for the relevant

6.2.4 Result summary

7 MONODOMAIN

8 CELLML MODEL

REFERENCES

[1] Chris Bradley, Andy Bowery, Randall Britten, Vincent Budelmann, Oscar Camara, Richard Christie, Andrew Cookson, Alejandro F Frangi, Thiranja Babarenda Gamage, Thomas Heidlauf, et al. Opencmiss: a multi-physics & multi-scale computational infrastructure for the vph/physiome project. Progress in biophysics and molecular biology, 107(1):32-47, 2011.